



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 5, 2020 – 04:08 PM JST

PDB ID : 7C7X
Title : Structural insights into nucleosome reorganization by NAP1-RELATED PROTEIN 1 (NRP1)
Authors : Luo, Q.; Baihui, W.
Deposited on : 2020-05-27
Resolution : 3.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.14.6
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.14.6

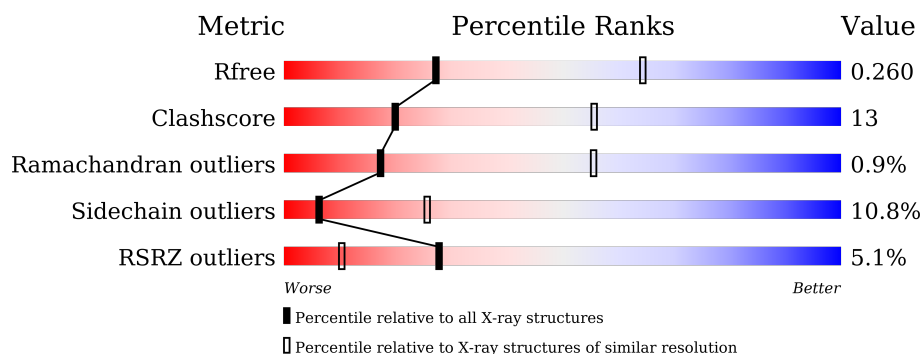
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	93	<div> <div>0%</div> <div> <div>62%</div> <div>23%</div> <div>•</div> <div>13%</div> </div> </div>
1	C	93	<div> <div>4%</div> <div> <div>57%</div> <div>28%</div> <div>•</div> <div>13%</div> </div> </div>
2	B	98	<div> <div>74%</div> <div>14%</div> <div>•</div> <div>7%</div> </div>
2	D	98	<div> <div>69%</div> <div>17%</div> <div>5%</div> <div>8%</div> </div>
3	E	239	<div> <div>5%</div> <div> <div>58%</div> <div>13%</div> <div>•</div> <div>27%</div> </div> </div>
3	F	239	<div> <div>8%</div> <div> <div>49%</div> <div>17%</div> <div>•</div> <div>31%</div> </div> </div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 5502 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Histone H2A.6.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	C	81	Total	C	N	O	0	0	0
			620	396	114	110			
1	A	81	Total	C	N	O	0	0	0
			615	393	112	110			

- Molecule 2 is a protein called Histone H2B.1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	90	Total	C	N	O	S	0	0	0
			707	455	120	130	2			
2	B	91	Total	C	N	O	S	0	0	0
			715	459	122	132	2			

- Molecule 3 is a protein called NAP1-related protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	174	Total	C	N	O	S	0	0	0
			1426	922	221	282	1			
3	F	166	Total	C	N	O	S	0	0	0
			1371	890	211	269	1			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	18	SER	-	expression tag	UNP Q9CA59
F	18	SER	-	expression tag	UNP Q9CA59

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	D	1	Total	C	O	0	0
			6	3	3		
4	D	1	Total	C	O	0	0
			6	3	3		
4	D	1	Total	C	O	0	0
			6	3	3		
4	F	1	Total	C	O	0	0
			6	3	3		

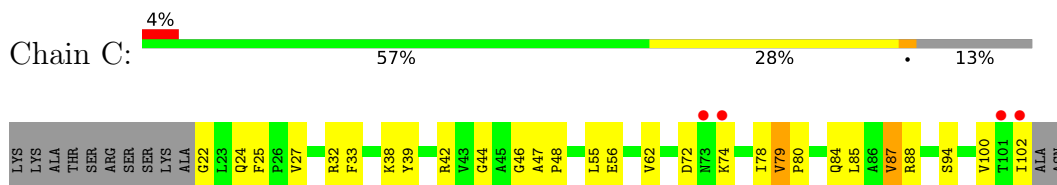
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	4	Total	O	0	0
			4	4		
5	D	3	Total	O	0	0
			3	3		
5	E	3	Total	O	0	0
			3	3		
5	F	5	Total	O	0	0
			5	5		
5	A	6	Total	O	0	0
			6	6		
5	B	3	Total	O	0	0
			3	3		

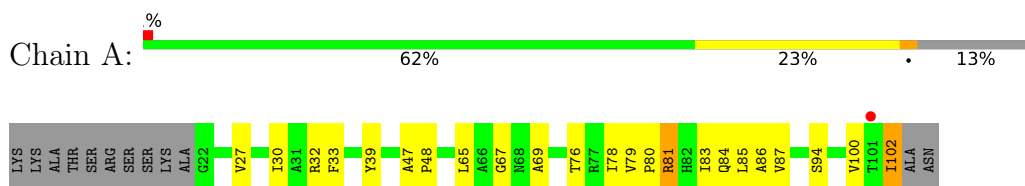
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

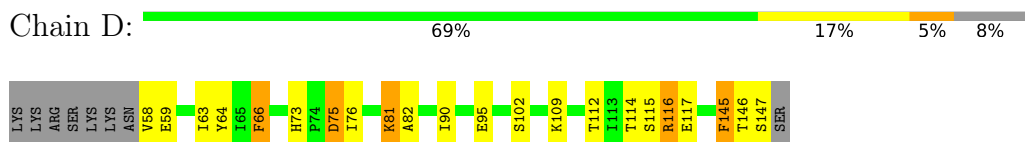
• Molecule 1: Histone H2A.6



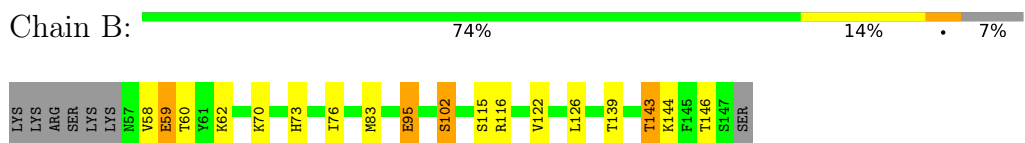
• Molecule 1: Histone H2A.6



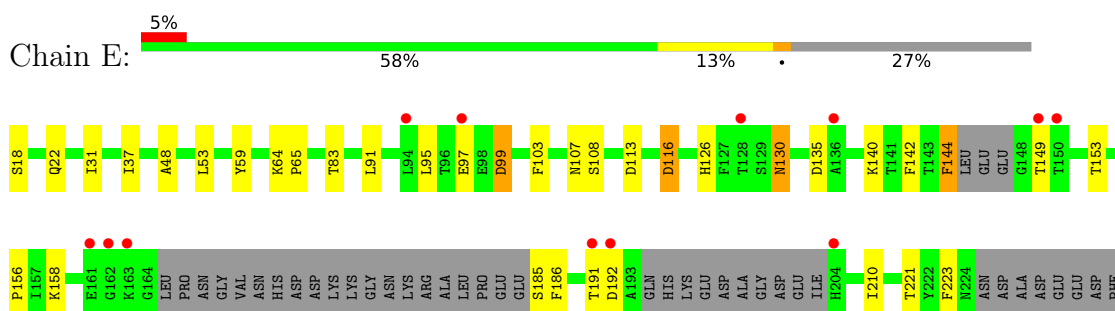
• Molecule 2: Histone H2B.1



• Molecule 2: Histone H2B.1



• Molecule 3: NAP1-related protein 1



ASP	GLY
ASP	ASP
ASP	ASP
ASP	GLY
ASP	ASP
GLU	GLU
GLU	GLY
GLU	GLY
GLU	ASP
ASP	ASP
ASP	ASP
ASP	ASP
GLU	GLU
GLU	GLU
GLU	ASP
GLY	GLU
GLU	GLU

● Molecule 3: NAP1-related protein 1



SER	ASN	LEU	E21	Q22	I23	D24	I31	E32	E36	D39	K47	A48	S49	L53	E54	V55	E56	Y59	V66	V73	F80	W81	F85	L91	G92	D93	L94	L95	T96	E97	E98	D99	Q100	I101	I102	F103	K104	Y105	L106	R107	S108	D113	D116	S119
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T128	S129	M130	F131	F132	F133	E134	F144	L145	E147	G148	T149	T150	K151	A154	K158	W159	K160	E161	GLY	LYS	GLY	LEU	PRO	ASN	GLY	VAL	ASN	HIS	ASP	ASP	LYS	LYS	GLY	ASN	LYS	ARG	ALA	LEU	PRO	GLU	SER	PHE	F187	F190	T191	ASP	ALA	GLN	HIS	LYS	GLU	ASP	ALA
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GLY	ASP	GLU	ILE	H204	D205	E206	S217	F223	N224	ASN	ASP	ALA	ASP	GLU	GLU	ASP	ASP	PHE	ASP	GLY	ASP	ASP	GLY	ASP	GLU	GLU	GLY	GLU	GLU	ASP	ASP	ASP	ASP	GLU	GLU	GLU	GLU	ASP	GLY	GLU	GLU	GLU	GLU	GLU	GLU	GLU
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4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	66.71Å 128.40Å 140.28Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.62 – 3.00 29.60 – 2.99	Depositor EDS
% Data completeness (in resolution range)	84.9 (29.62-3.00) 84.2 (29.60-2.99)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.10 (at 3.00Å)	Xtriage
Refinement program	REFMAC 5.8.0253	Depositor
R, R_{free}	0.223 , 0.262 0.227 , 0.260	Depositor DCC
R_{free} test set	1044 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	54.9	Xtriage
Anisotropy	0.201	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 68.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.39$, $\langle L^2 \rangle = 0.21$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	5502	wwPDB-VP
Average B, all atoms (Å ²)	80.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.97% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.73	1/622 (0.2%)	0.85	0/840
1	C	0.70	0/628	0.84	0/848
2	B	0.70	0/726	0.87	0/976
2	D	0.71	0/718	0.90	0/965
3	E	0.71	0/1457	0.86	1/1969 (0.1%)
3	F	0.67	0/1401	0.82	0/1895
All	All	0.70	1/5552 (0.0%)	0.85	1/7493 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	69	ALA	C-O	5.64	1.34	1.23

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	192	ASP	CB-CG-OD2	5.16	122.94	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	615	0	647	31	0
1	C	620	0	652	21	0
2	B	715	0	753	11	0
2	D	707	0	747	23	0
3	E	1426	0	1382	19	0
3	F	1371	0	1333	55	0
4	D	18	0	24	2	0
4	F	6	0	8	0	0
5	A	6	0	0	2	0
5	B	3	0	0	0	0
5	C	4	0	0	1	0
5	D	3	0	0	1	0
5	E	3	0	0	1	0
5	F	5	0	0	2	0
All	All	5502	0	5546	139	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 13.

All (139) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:132:PHE:O	3:F:160:LYS:N	1.81	1.14
3:F:131:PRO:O	3:F:160:LYS:HB3	1.51	1.10
1:A:81:ARG:HD2	1:A:102:ILE:HD11	1.33	1.09
3:F:131:PRO:O	3:F:160:LYS:CB	1.99	1.09
3:F:95:LEU:HD11	3:F:103:PHE:CE2	1.93	1.02
1:A:80:PRO:HB3	1:A:102:ILE:HG23	1.46	0.95
1:A:81:ARG:HD2	1:A:102:ILE:CD1	1.95	0.95
5:A:201:HOH:O	2:B:59:GLU:HG3	1.69	0.93
1:A:80:PRO:CB	1:A:102:ILE:HG23	2.04	0.88
3:F:147:GLU:OE1	3:F:147:GLU:N	2.08	0.86
3:F:47:LYS:HD3	5:F:403:HOH:O	1.75	0.86
1:C:39:TYR:O	2:D:102:SER:OG	2.00	0.80
1:A:81:ARG:CD	1:A:102:ILE:CD1	2.63	0.76
2:D:147:SER:O	5:D:301:HOH:O	2.05	0.74
3:F:131:PRO:O	3:F:160:LYS:HD2	1.88	0.74
1:A:81:ARG:CD	1:A:102:ILE:HD11	2.15	0.74
1:A:84:GLN:NE2	1:A:100:VAL:O	2.21	0.73
3:F:131:PRO:O	3:F:160:LYS:CD	2.35	0.73
2:B:139:THR:O	2:B:143:THR:OG1	2.07	0.73
3:F:131:PRO:O	3:F:160:LYS:HB2	1.89	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:301:HOH:O	2:B:62:LYS:HD2	1.91	0.70
3:F:134:GLU:HG3	3:F:160:LYS:HE3	1.72	0.70
1:A:39:TYR:O	2:B:102:SER:OG	2.09	0.69
3:E:156:PRO:HG2	3:E:158:LYS:HE2	1.76	0.68
3:E:135:ASP:OD2	3:E:158:LYS:HG3	1.95	0.67
3:E:135:ASP:OD1	3:E:158:LYS:HE3	1.94	0.66
3:F:95:LEU:HD11	3:F:103:PHE:CZ	2.29	0.66
3:E:130:ASN:HD22	3:E:130:ASN:N	1.93	0.65
1:A:80:PRO:HB2	1:A:102:ILE:CG2	2.26	0.65
1:A:80:PRO:CB	1:A:102:ILE:CG2	2.73	0.65
2:D:66:PHE:CD2	4:D:201:GOL:O3	2.49	0.65
3:F:134:GLU:CG	3:F:160:LYS:HE3	2.28	0.64
3:E:116:ASP:OD1	3:E:116:ASP:N	2.31	0.63
3:F:94:LEU:N	3:F:94:LEU:HD23	2.13	0.62
3:F:96:THR:N	3:F:99:ASP:OD2	2.29	0.62
2:D:146:THR:HG22	2:D:146:THR:O	2.01	0.61
3:F:101:LYS:HE2	3:F:105:TYR:HE2	1.65	0.61
1:A:39:TYR:OH	2:B:95:GLU:OE1	2.20	0.60
1:A:81:ARG:CD	1:A:102:ILE:HD12	2.31	0.60
3:E:135:ASP:CG	3:E:158:LYS:HE3	2.21	0.60
1:C:33:PHE:CZ	2:D:59:GLU:HG2	2.37	0.59
3:F:95:LEU:HD11	3:F:103:PHE:CD2	2.37	0.59
3:E:144:PHE:HA	3:E:149:THR:O	2.02	0.58
1:C:22:GLY:HA2	2:D:145:PHE:CZ	2.38	0.58
2:D:114:THR:OG1	2:D:116:ARG:HB2	2.03	0.58
1:A:81:ARG:HE	1:A:85:LEU:HD11	1.69	0.58
3:F:47:LYS:CD	5:F:403:HOH:O	2.41	0.57
1:A:76:THR:O	2:B:76:ILE:HG23	2.06	0.56
3:F:101:LYS:CE	3:F:105:TYR:HE2	2.19	0.56
3:E:64:LYS:HB3	3:E:65:PRO:HD3	1.88	0.55
3:E:135:ASP:OD2	3:E:158:LYS:HE3	2.06	0.55
3:E:48:ALA:HA	3:F:59:TYR:CE2	2.42	0.54
1:A:84:GLN:O	1:A:87:VAL:HG22	2.07	0.54
3:F:132:PHE:O	3:F:160:LYS:CB	2.56	0.54
3:F:134:GLU:CD	3:F:160:LYS:HE3	2.27	0.54
1:C:42:ARG:NH2	2:D:117:GLU:OE2	2.41	0.53
2:B:73:HIS:HB3	2:B:76:ILE:HD12	1.91	0.53
3:E:108:SER:HB3	3:E:126:HIS:HB2	1.90	0.53
1:A:79:VAL:HG23	1:A:81:ARG:H	1.73	0.53
1:C:84:GLN:NE2	1:C:102:ILE:HD12	2.23	0.52
3:F:85:PHE:CE1	3:F:91:LEU:HB3	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:95:LEU:CD1	3:F:103:PHE:CD2	2.92	0.52
3:F:106:LEU:HG	3:F:106:LEU:O	2.09	0.52
3:F:132:PHE:CD1	3:F:132:PHE:N	2.72	0.52
1:A:85:LEU:H	1:A:85:LEU:HD12	1.76	0.51
3:F:53:LEU:HA	3:F:56:GLU:HG3	1.93	0.51
1:C:32:ARG:HD3	5:C:204:HOH:O	2.11	0.51
3:F:105:TYR:CE1	3:F:129:SER:O	2.64	0.51
3:F:95:LEU:CD1	3:F:103:PHE:CE2	2.82	0.51
3:F:81:TRP:CD1	3:F:108:SER:HA	2.46	0.51
3:F:150:THR:OG1	3:F:151:LYS:N	2.42	0.51
1:A:80:PRO:HB2	1:A:102:ILE:HG21	1.93	0.50
1:C:62:VAL:O	1:C:62:VAL:HG12	2.10	0.50
1:C:79:VAL:HA	2:D:82:ALA:HB2	1.94	0.50
3:F:132:PHE:O	3:F:160:LYS:CA	2.58	0.50
2:B:62:LYS:HG2	2:B:83:MET:HG3	1.94	0.49
1:C:44:GLY:O	1:C:46:GLY:N	2.44	0.49
2:D:63:ILE:HD11	3:F:32:GLU:HB3	1.95	0.49
3:F:131:PRO:O	3:F:160:LYS:CG	2.60	0.49
1:A:33:PHE:CE1	2:B:59:GLU:HG2	2.47	0.49
1:A:79:VAL:O	1:A:80:PRO:C	2.51	0.49
3:E:59:TYR:CD1	3:F:48:ALA:HB2	2.47	0.49
3:F:132:PHE:O	3:F:160:LYS:HB2	2.13	0.48
3:F:101:LYS:CE	3:F:105:TYR:CE2	2.96	0.48
1:A:81:ARG:HD3	1:A:102:ILE:HD12	1.95	0.48
3:E:99:ASP:N	3:E:99:ASP:OD1	2.45	0.47
3:F:131:PRO:HA	3:F:160:LYS:HD2	1.96	0.47
3:F:96:THR:HG22	3:F:97:GLU:H	1.79	0.47
1:A:30:ILE:HA	1:A:33:PHE:CD2	2.50	0.47
1:A:47:ALA:N	1:A:48:PRO:HD2	2.30	0.47
1:C:80:PRO:CG	2:D:81:LYS:HD3	2.44	0.47
3:F:101:LYS:HD2	3:F:101:LYS:O	2.15	0.47
1:A:83:ILE:O	1:A:86:ALA:HB3	2.15	0.47
1:A:81:ARG:HA	1:A:102:ILE:HD11	1.96	0.46
3:E:95:LEU:HD11	3:E:103:PHE:CE2	2.50	0.46
1:C:78:ILE:HG13	2:D:76:ILE:HG21	1.96	0.46
1:C:33:PHE:CE2	2:D:59:GLU:HG2	2.51	0.46
3:F:133:PHE:HB2	3:F:158:LYS:O	2.16	0.46
3:F:116:ASP:OD1	3:F:119:SER:OG	2.32	0.46
3:F:36:GLU:O	3:F:39:ASP:HB2	2.15	0.46
1:A:32:ARG:HD3	5:A:203:HOH:O	2.16	0.45
1:C:25:PHE:CE1	1:C:56:GLU:HA	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:185:SER:OG	3:E:186:PHE:N	2.50	0.45
1:A:81:ARG:HD2	1:A:81:ARG:HA	1.37	0.45
3:F:133:PHE:HD1	3:F:133:PHE:O	1.99	0.45
1:A:67:GLY:HA2	1:A:78:ILE:HD11	1.99	0.44
1:C:22:GLY:HA2	2:D:145:PHE:HZ	1.79	0.44
1:C:27:VAL:HG13	1:C:48:PRO:HB2	1.99	0.44
3:F:130:ASN:HA	3:F:131:PRO:HD3	1.87	0.44
2:D:73:HIS:C	2:D:75:ASP:H	2.21	0.44
3:F:130:ASN:OD1	3:F:132:PHE:CD1	2.70	0.44
2:D:109:LYS:HG3	2:D:109:LYS:O	2.18	0.44
3:F:132:PHE:C	3:F:160:LYS:HB2	2.38	0.43
1:C:24:GLN:O	2:D:64:TYR:HD2	2.02	0.43
3:F:131:PRO:HA	3:F:160:LYS:CD	2.47	0.43
2:B:122:VAL:HG13	2:B:126:LEU:HD12	2.01	0.43
3:F:130:ASN:OD1	3:F:132:PHE:HD1	2.01	0.43
3:F:101:LYS:HE3	3:F:105:TYR:CE2	2.53	0.43
2:D:63:ILE:HD11	3:F:32:GLU:CB	2.48	0.43
3:F:80:PHE:HA	3:F:223:PHE:CE1	2.53	0.43
1:A:27:VAL:HG12	2:B:146:THR:HG23	2.00	0.42
1:A:81:ARG:HA	1:A:102:ILE:CD1	2.50	0.42
3:E:91:LEU:HD11	3:E:210:ILE:HG22	2.01	0.42
2:D:73:HIS:HB3	2:D:76:ILE:HD12	2.01	0.42
1:C:79:VAL:HB	1:C:80:PRO:HD2	2.02	0.42
3:F:160:LYS:O	3:F:161:GLU:O	2.37	0.41
1:C:55:LEU:HD22	2:D:90:ILE:HG23	2.02	0.41
3:F:101:LYS:C	3:F:101:LYS:HD2	2.41	0.41
2:D:66:PHE:HD2	4:D:201:GOL:HO3	1.57	0.41
3:E:135:ASP:OD1	3:E:158:LYS:CE	2.67	0.41
3:F:24:ASP:OD1	3:F:24:ASP:C	2.59	0.41
1:C:87:VAL:HG12	1:C:88:ARG:N	2.36	0.41
1:A:79:VAL:HB	1:A:80:PRO:HD2	2.02	0.41
3:E:130:ASN:ND2	3:E:130:ASN:N	2.66	0.40
3:E:140:LYS:HE2	3:E:142:PHE:CZ	2.56	0.40
1:C:78:ILE:HG13	2:D:76:ILE:CG2	2.51	0.40
3:F:103:PHE:O	3:F:106:LEU:HB3	2.21	0.40
1:C:47:ALA:N	1:C:48:PRO:HD2	2.37	0.40
2:D:145:PHE:HD1	2:D:145:PHE:O	2.05	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	79/93 (85%)	69 (87%)	10 (13%)	0	100	100
1	C	79/93 (85%)	65 (82%)	11 (14%)	3 (4%)	3	18
2	B	89/98 (91%)	83 (93%)	5 (6%)	1 (1%)	14	50
2	D	88/98 (90%)	81 (92%)	7 (8%)	0	100	100
3	E	166/239 (70%)	141 (85%)	23 (14%)	2 (1%)	13	48
3	F	158/239 (66%)	133 (84%)	25 (16%)	0	100	100
All	All	659/860 (77%)	572 (87%)	81 (12%)	6 (1%)	17	55

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	E	223	PHE
1	C	100	VAL
1	C	74	LYS
2	B	70	LYS
3	E	37	ILE
1	C	87	VAL

5.3.2 Protein sidechains

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	60/70 (86%)	56 (93%)	4 (7%)	16	49
1	C	61/70 (87%)	56 (92%)	5 (8%)	11	39

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	80/87 (92%)	71 (89%)	9 (11%)	6	24
2	D	79/87 (91%)	70 (89%)	9 (11%)	5	24
3	E	159/214 (74%)	144 (91%)	15 (9%)	8	32
3	F	153/214 (72%)	131 (86%)	22 (14%)	3	15
All	All	592/742 (80%)	528 (89%)	64 (11%)	6	26

All (64) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	38	LYS
1	C	72	ASP
1	C	79	VAL
1	C	85	LEU
1	C	94	SER
2	D	58	VAL
2	D	66	PHE
2	D	75	ASP
2	D	81	LYS
2	D	95	GLU
2	D	112	THR
2	D	115	SER
2	D	116	ARG
2	D	145	PHE
3	E	18	SER
3	E	22	GLN
3	E	31	ILE
3	E	53	LEU
3	E	83	THR
3	E	97	GLU
3	E	99	ASP
3	E	107	ASN
3	E	113	ASP
3	E	116	ASP
3	E	130	ASN
3	E	144	PHE
3	E	153	THR
3	E	191	THR
3	E	221	THR
3	F	22	GLN
3	F	23	ILE
3	F	31	ILE

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Mol	Chain	Res	Type
3	F	49	SER
3	F	53	LEU
3	F	54	GLU
3	F	66	VAL
3	F	73	VAL
3	F	93	ASP
3	F	94	LEU
3	F	99	ASP
3	F	113	ASP
3	F	116	ASP
3	F	119	SER
3	F	130	ASN
3	F	132	PHE
3	F	133	PHE
3	F	134	GLU
3	F	144	PHE
3	F	151	LYS
3	F	206	GLU
3	F	217	SER
1	A	65	LEU
1	A	81	ARG
1	A	94	SER
1	A	102	ILE
2	B	58	VAL
2	B	59	GLU
2	B	60	THR
2	B	95	GLU
2	B	102	SER
2	B	115	SER
2	B	116	ARG
2	B	143	THR
2	B	144	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
2	D	73	HIS
3	E	22	GLN
3	E	107	ASN
3	E	130	ASN
3	F	100	GLN
3	F	130	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	GOL	D	203	-	5,5,5	0.65	0	5,5,5	0.45	0
4	GOL	D	201	-	5,5,5	0.09	0	5,5,5	0.37	0
4	GOL	F	301	-	5,5,5	0.57	0	5,5,5	0.47	0
4	GOL	D	202	-	5,5,5	0.58	0	5,5,5	0.36	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	D	203	-	-	1/4/4/4	-
4	GOL	D	201	-	-	2/4/4/4	-
4	GOL	F	301	-	-	4/4/4/4	-
4	GOL	D	202	-	-	0/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	201	GOL	O1-C1-C2-C3
4	F	301	GOL	C1-C2-C3-O3
4	F	301	GOL	O1-C1-C2-C3
4	D	201	GOL	O1-C1-C2-O2
4	F	301	GOL	O1-C1-C2-O2
4	F	301	GOL	O2-C2-C3-O3
4	D	203	GOL	C1-C2-C3-O3

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	201	GOL	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	81/93 (87%)	-0.27	1 (1%) 79 54	25, 65, 118, 144	0
1	C	81/93 (87%)	-0.22	4 (4%) 29 11	25, 63, 119, 154	0
2	B	91/98 (92%)	-0.53	0 100 100	25, 52, 94, 105	0
2	D	90/98 (91%)	-0.54	0 100 100	26, 52, 93, 115	0
3	E	174/239 (72%)	0.13	12 (6%) 16 5	39, 89, 156, 184	0
3	F	166/239 (69%)	0.24	18 (10%) 5 2	43, 93, 167, 190	0
All	All	683/860 (79%)	-0.11	35 (5%) 28 10	25, 71, 152, 190	0

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	F	147	GLU	6.2
3	E	161	GLU	4.8
3	E	162	GLY	4.2
1	C	73	ASN	4.1
3	F	150	THR	3.9
3	E	192	ASP	3.7
3	F	98	GLU	3.2
3	E	150	THR	3.1
3	F	97	GLU	3.0
3	F	151	LYS	2.9
3	F	149	THR	2.7
3	F	191	THR	2.7
3	F	159	TRP	2.7
3	E	97	GLU	2.6
3	E	128	THR	2.6
3	E	136	ALA	2.6
3	E	163	LYS	2.5
3	E	94	LEU	2.4
3	F	190	PHE	2.4

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Mol	Chain	Res	Type	RSRZ
3	F	92	GLY	2.3
3	F	160	LYS	2.3
1	C	102	ILE	2.3
3	F	23	ILE	2.3
1	C	74	LYS	2.2
3	F	161	GLU	2.2
3	F	128	THR	2.2
3	F	204	HIS	2.2
1	A	101	THR	2.2
3	F	99	ASP	2.2
3	E	149	THR	2.2
1	C	101	THR	2.2
3	E	204	HIS	2.2
3	F	101	LYS	2.1
3	F	154	ALA	2.1
3	E	191	THR	2.1

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	GOL	D	203	6/6	0.83	0.21	28,31,31,31	0
4	GOL	D	202	6/6	0.92	0.27	28,30,30,30	0
4	GOL	D	201	6/6	0.94	0.22	53,57,59,61	0
4	GOL	F	301	6/6	0.95	0.30	30,32,32,32	0

6.5 Other polymers [i](#)

There are no such residues in this entry.